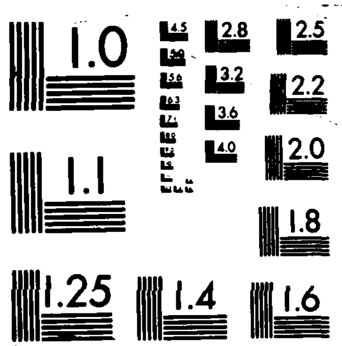
AD-A174 648 ON FIRST PASSAGE TIMES AND DIFFERENTIAL EQUATIONS(U) 1/1
FORD AEROSPACE AND COMMUNICATIONS CORP PALO ALTO CA
M L WENOCUR 1986 AFOSR-TR-86-0478 F49620-86-C-0022

UNCLASSIFIED F/G 12/1 NL



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AFOSR-TR- 86-0478

On First Passage Times and Differential Equations

By
Michael L. Wenocur
Ford Aerospace and Communications Corporation
Palo Alto, California

Practical and theoretical considerations in computing first passage time statistics are considered. We are motivated by first passage times as models of failure times.

In particular, let $X(t)$ be a diffusion on $[0,r]$ with a reflecting boundary at 0. Denote by τ_r the time of first passage to level r, ie, $\tau_r = inf\{t > 0 , X(t) \geq r\}$, and let $w(x,t)$ be its tail probability function conditional on $X(0) = 0$, ie $w(x,t) = P\{\tau_r > t \mid X(0) = x\} \equiv P^x\{\tau_r > t\}$.

In Section 1, the relevance of first passage time distributions as failure time models is indicated (cf [8]). Also, the spectral series expansion solution to the backward equation is introduced.

In Section 2, algorithms for approximating $w(x,t)$ are obtained. In particular, the infinite spectral expansion for $w(x,t)$ is approximated by an n-term sub-expansion which matches the first $n-1$ moments. Proofs validating the spectral expansion and the related approximation scheme are given in the Appendix.

In Sections 3 and 4, methods are given for obtaining the eigenvalues and first passage moments, necessary for computing approximations to $w(x,t)$. In Section 5, computational issues related to calculating the moment generating function are considered.

Sections 6 and 7 include theoretical complements about first passage times. In particular, the moment generating function is shown to possess an interesting representation having exponential form (cf equation (7.1)). This exponential representation is related to asymptotic expansions used in analyzing perturbations of certain second-order differential equations.

This research was supported in part by Air Force Office of Scientific Research Contract F49620-86-C-0022.

REPORT DOCUMENTATION PAGE

1a. REPORT SECURITY CLASSIFICATION Unclassified	1b. RESTRICTIVE MARKINGS AD-A174 648
2a. SECURITY CLASSIFICATION AUTHORITY 2b. DECLASSIFICATION/DOWNGRADING SCHEDULE	3. DISTRIBUTION/AVAILABILITY OF REPORT Approved for public release; distribution unlimited.
4. PERFORMING ORGANIZATION REPORT NUMBER(S)	5. MONITORING ORGANIZATION REPORT NUMBER(S) AFOSR-TR- 86-0478
6a. NAME OF PERFORMING ORGANIZATION Ford Aerospace and Communications Corporation 6b. OFFICE SYMBOL (If applicable)	7a. NAME OF MONITORING ORGANIZATION AFOSR/NM
6c. ADDRESS (City, State and ZIP Code) Ford Aerospace and Communications Corporation Palo Alto, CA	7b. ADDRESS (City, State and ZIP Code) Bldg. 410 Bolling AFB, DC 20332-6448
8a. NAME OF FUNDING/SPONSORING ORGANIZATION AFOSR 8b. OFFICE SYMBOL (If applicable) NM	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER F49620-86-C-0022
8c. ADDRESS (City, State and ZIP Code) Bolling Air Force Base Washington, DC 20332-6448	10. SOURCE OF FUNDING NOS. PROGRAM ELEMENT NO.: 61102F PROJECT NO.: 2304 TASK NO.: A5 WORK UNIT NO.:
11. TITLE (Include Security Classification) "On First Passage Times and Differential Equations"	
12. PERSONAL AUTHOR(S) Micheal L. Wenocur	
13a. TYPE OF REPORT reprint 13b. TIME COVERED FROM ______ TO ______	14. DATE OF REPORT (Yr., Mo., Day) 15. PAGE COUNT 24 (twenty-four)
16. SUPPLEMENTARY NOTATION	

17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
FIELD	GROUP	SUB. GR.	

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

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In particular, let $X(t)$ be a diffusion on $[0,r]$ with a reflecting boundary at 0. Denote by τ_r the time of first passage to level r, ie, $\tau_r = inf\{t > 0 , X(t) \geq r\}$, and let $w(x,t)$ be its tail probability function conditional on $X(0) = 0$, ie $w(x,t) = P\{ \tau_r > t \mid X(0) = x\} \equiv P^x\{\tau_r > t\}$.

20. DISTRIBUTION/AVAILABILITY OF ABSTRACT UNCLASSIFIED/UNLIMITED ☒ SAME AS RPT. ☐ DTIC USERS ☐	21. ABSTRACT SECURITY CLASSIFICATION Unclassified
22a. NAME OF RESPONSIBLE INDIVIDUAL Capt Woodruff	22b. TELEPHONE NUMBER (Include Area Code) 767-5025 22c. OFFICE SYMBOL NM

1. Introduction And Motivation

Let $\{\Omega , F , P\}$ be a probability space. Suppose that F_t is a filtration of F and that $\{W(t),\ t \geq 0\}$ is standard Brownian motion adapted to F_t.

Let

$$A \equiv \frac{\sigma^2(x)}{2} D^2 + \mu(x) D \tag{1.1}$$

be the infinitesimal generator of a diffusion $X(t)$ on $[0 , r]$ satisfying

$$dX(t) = \sigma(x) dW(t) + \mu(x) dt ,$$

with a reflecting boundary at 0 and absorption at $r < \infty$, and where $\sigma^2(x) > 0$ and $\mu(x)$ are continuously differentiable on $[0 , r]$.

Define the stopping time τ_r by

$$\tau_r \equiv inf \{s\colon s \geq 0 , X(s) \geq r\}$$

and the moment generating function $\Psi_\theta(x,y)$ by

$$\Psi_\theta(x,y) = E\{e^{\theta\tau_y} \mid X(0) = x\} \equiv E^x[e^{\theta\tau_y}]$$

1.1 First Passage Times As Failure Times

Our motivation for studying first passage time distributions is their relevance to modeling of failure times. Indeed, this paper continues the line of development initiated in [8], where a stochastic process is used to model system state, ie, *wear-and-tear*, and failure occurs when either a traumatic killing event occurs (killing events happen with rate $k(x)$ in state x), or the system is retired when *wear-and-tear* reaches some predefined threshold (ie, a first passage occurs).

For example, if system state is modeled as Brownian motion with positive drift, then first passage to a specified threshhold has an inverse Gaussian distribution. This first passage distribution has been successfully applied to numerous problems to obtain good fits, (cf Jorgensen [4]).

A related but parallel line of development is explored in Wenocur [11] , where the killing time distribution of Brownian motion with quadratic killing rate is calculated.

Our aim in this paper is to study first passage time distributions, where the system state process is a general diffusion with reflection at the origin and absorption at $r < \infty$. That is, the system state evolves as a diffusion, and failure occurs at the epoch of first passage (or absorption) to level r .

In future work, we intend to explore the practical ramifications of employing the computational methods suggested here to evaluate interesting first passage times statistics.

1.2 Backward Equation For First Passage Time Distribution

Let $w(x,t)$ denote the tail of the first passage time distribution, ie,

$$w(x,t) \equiv P^x\{\tau_r > t\} .$$

The backward differential equation for $w(x,t)$ is

$$\frac{\partial w(x,t)}{\partial t} = \mu(x)\frac{\partial w(x,t)}{\partial x} + \frac{\sigma^2(x)}{2}\frac{\partial^2 w(x,t)}{\partial x^2} = Aw(x,t) \tag{1.2}$$

for $(x,t) \in (0,r) \times (0,\infty)$, with boundary conditions

$$w(x,0) = 1 \text{ for } 0 < x < r \text{ , and for } \textit{all } t > 0 \;\; w(r,t) = 0 \text{ and } \frac{\partial w(0,t)}{\partial x} = 0 .$$

For a derivation of this equation and other related quantities see [5], pp 222-224.

1.3 The Spectral Representation for w(x,t)

The following representation for $w(x,t)$ is valid whenever $\sigma^2(x)$ and $\mu(x)$ are sufficiently smooth.

$$w(x,t) = \sum_{k=1}^{\infty} c_k \, e^{-\alpha_k t} \phi_k(x) \tag{1.3}$$

where α_k and ϕ_k are eigenvalues and eigenfunctions, and c_k are generalized *Fourier* coefficients, all defined below (This representation is proved in Section 8.1).

The $\{\phi_k , k \geq 1\}$ are eigenfunctions of A corresponding to the eigenvalues $\{\alpha_k , k \geq 1\}$, ie,

$$A\phi_k = -\alpha_k \phi_k ,$$

and

$$c_k = \int_0^r \phi_k(x)\rho(x)dx ,$$

where $\rho(x)$ is given by

$$\rho(x) = 2\pi(x)/\sigma^2(x) \tag{1.4}$$

and $\pi(x)$ is given by

$$\pi(x) = \exp\int_0^x 2\mu(u)/\sigma^2(u)du \ . \tag{1.5}$$

In general an arbitrary function $f \in L^2(\rho)$ will have a *Fourier* type expansion, ie,

$$f = \sum_{k=1}^{\infty} c_k \phi_k$$

where equality is interpreted in the $L^2(\rho)$ sense and

$$c_k = \int_0^r f(x)\phi_k(x)\rho(x)dx$$

Remark: In the sequel it is assumed that A's eigenvalues form a complete set in $L^2(\rho)$. The completeness of A's eigenfunctions can be assured by certain regularity conditions on the infinitesimal parameters $\sigma^2(x)$ and $\mu(x)$. For example, $\sigma^2(x) > 0$ and the continuity of $\sigma^{2''}(x)$ and $\mu'(x)$ are sufficient conditions. See [10, chap 1] for more details.

1.4 A Generalization

This paper is primarily concerned with computing first passage time statistics. In [8], as alluded to in (1.1), a general reliability model was proposed in which system failures occur when either system wear-and-tear reaches some maximum permissible level (ie, a first passage occurs) , or when some killing event happens (such killing events occur with rate $k(x)$ in state x). Under this model $w(x,t)$ satisfies the following equation:

$$\frac{\partial w(x,t)}{\partial t} = k(x)w(x,t)\mu(x)\frac{\partial w(x,t)}{\partial x} + \frac{\sigma^2(x)}{2}\frac{\partial^2 w(x,t)}{\partial x^2} = Bw(x,t) \ ,$$

with the same boundary conditions as (1.2) , and where

$$Bf(x) = \frac{1}{2}\sigma^2(x)f''(x) + \mu(x)f'(x) + k(x)f(x) \ .$$

It is possible to solve for $w(x,t)$ and related quantities with methods very similar to those presented here.

Acknowledgement. I gladly thank A. Lemoine for his unflagging encouragement while this work was in progress, and for his expert editorial help which immensely improved the readability of this work.

2. Approximating The First Passage Time Distribution

The above discussion might suggest that solving for $w(x,t)$ is pretty straightforward. But generally eigenvalues and especially eigenfunctions are difficult to obtain. However the problem of approximating $w(x,t)$ can be approached by the method of moments. One technique is to calculate the first three moments, and then use the Pearson curve fitting method (cf [9]). This method is computationally feasible, and the Pearson family of curves includes some important first passage distributions, such as the gamma distribution (cf [1]). The merits of this approach will be studied in a forthcoming paper.

2.1 Given n Eigenvalues And $n-1$ First Passage Moments

A more computationally intensive approach, but one founded on stronger theoretical grounds, is the following. Suppose that n moments $\{M_k(x,r)\ ,\ 1 \le k \le n\ \}$ are known, where $M_k(x,r) = E^x[\ \tau_r^k\ ]$, as well as the first n eigenvalues $\{\alpha_k\ ,\ 1 \le k \le n\ \}$. Then use a finite sum in place of the infinite sum in equation (1.3). In particular, approximate $w(x,t)$ by

$$w_n(x,t) = \sum_{j=1}^{n} p_j^{(n)}(x)\ e^{-t/\mu_j}$$

where $\mathbf{p}^{(n)} \equiv (p_1^{(n)}\ , \ . \ . \ . \ , p_n^{(n)})$ satisfies for $0 \le k \le n-1$

$$\sum_{j=1}^{n} p_j^{(n)}(x)\ (\mu_j)^k = \frac{M_k(x,r)}{k!} \quad where \quad \mu_j = 1/\alpha_j \tag{2.1}$$

Ideally we want $w_n(x,t)$ to be a distribution function, ie, $w_n(x,t) \ge 0$ and $w_n(x,s+t) \ge w_n(x,t)$ whenever $s > 0$. It is not clear that solving (2.1) always produces such a function. This issue requires further investigation.

2.1.1 Obtaining The Weighting Factors

The weighting factors $\{p_k^{(n)}\ ,\ 1 \le k \le n\ \}$ in (2.1) above are obtained by solving the following linear system:

$$\begin{bmatrix} 1 & 1 & \cdots & 1 \\ \mu_1 & \mu_2 & \cdots & \mu_N \\ \mu_1^2 & \mu_2^2 & \cdots & \mu_N^2 \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ \mu_1^{n-1} & \mu_2^{n-1} & \cdots & \mu_N^{n-1} \end{bmatrix} \begin{bmatrix} p_1^{(n)} \\ p_2^{(n)} \\ \cdot \\ \cdot \\ p_n^{(n)} \end{bmatrix} = \begin{bmatrix} 1 \\ m_1 \\ m_2 \\ \cdot \\ \cdot \\ m_{n-1} \end{bmatrix} \tag{2.2}$$

where $\mu_j = 1/\alpha_j$ and $m_k = M_k(x,r)/k!$

Observe that the matrix $\{\mu_j^k, 1 \leq j \leq n, 0 \leq j < n\}$ is none other than the transpose of the celebrated Vandermonde matrix. Cramer's equation gives the following formula for $p_k^{(n)}$.

$$p_k^{(n)} = \sum_{1 \leq j \leq n} m_j g_{n-j}(\mu_1, \mu_2, \cdots, \mu_{k-1}, \mu_{k+1}, \cdots \mu_n) \Big/ \prod_{\substack{1 \leq j \leq n \\ j \neq k}} (\mu_j - \mu_k) \qquad (2.3)$$

where g_r are the signed symmetric functions defined as follows:

$$g_0(a_1, a_2, \cdots, a_m) = 1$$

and for $r \geq 1$

$$g_r(a_1, a_2, \cdots, a_m) = \sum_{1 \leq i_1 < i_2 < \cdots < i_r \leq m} a_{i_1} a_{i_2} \cdots a_{i_r} (-1)^r$$

It is shown in Section (8.2) that $p_k^{(n)} - p_k = O(n^{-2})$.

2.2 Given $2n-1$ Moments Only

Suppose that the first $2n-1$ moments have been determined. It is possible to approximately determine the first n eigenvalues by solving the following system of equations for μ_i , $1 \leq i \leq n$.

$$\begin{bmatrix} 1 & 1 & \cdots & 1 \\ \mu_1 & \mu_2 & \cdots & \mu_n \\ \mu_1^2 & \mu_2^2 & \cdots & \mu_n^2 \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ \mu_1^{2n-1} & \mu_2^{2n-1} & \cdots & \mu_n^{2n-1} \end{bmatrix} \begin{bmatrix} p_1^{(n)} \\ p_2^{(n)} \\ \cdot \\ p_n^{(n)} \end{bmatrix} = \begin{bmatrix} 1 \\ m_1 \\ m_2 \\ \cdot \\ \cdot \\ m_{2n-1} \end{bmatrix}$$

where $\mu_j > 0$.

One approach is to solve for $\mathbf{p}^{(n)}$ in terms of $\{\mu_k , 1 \leq k \leq n\}$ and $\{m_0 , m_1 , \cdots , m_{n-1}\}$ as detailed above, and then use the remaining n constraints to determine the $\{\mu_k , 1 \leq k \leq n\}$. This reduced system can then be solved using mathematical programming techniques, eg, approximate Newton-Raphson techniques. The numerical stability and feasibility of this method merit further study.

3. Solving For The Eigenvalues

3.1 The Eigenvalue Equation

Before the eigenvalue equation can be introduced, the eigenfunction differential equation must be rewritten in more suitable form. To do so, let $Y_\theta(x)$ satisfy

$$\frac{1}{2}\sigma^2(x)Y_\theta''(x) + \mu(x)Y_\theta'(x) + \theta Y_\theta(x) = 0 \tag{3.1}$$

Multiplying (3.1) by $\rho(x)$ gives

$$\pi(x)Y_\theta''(x) + \pi'(x)Y_\theta'(x) + \theta\rho(x)Y_\theta(x) \ , \tag{3.2}$$

where $\rho(x)$ and $\pi(x)$ are given by (1.4) and (1.5) respectively.

Now suppose that Y_θ satisfies the boundary conditions

$Y_\theta'(0) = 0$ and $Y_\theta(0) = 1$

Then define $\omega(\theta)$ by

$$\omega(\theta) = Y_\theta(r) \tag{3.3}$$

The eigenvalues of equation (3.1) are none other than the zeroes of ω, see [2, Chap 8] for further details.

3.2 Standardized Eigenvalue Problem

It is also possible to transform (3.1) into more standard form using the following transformation scheme.

setting $z = Z(x) = \int_0^x \frac{du}{(\sigma^2(u)/2)^{1/2}}$ reduces (3.1) to

$$\frac{d^2Y}{dz^2} + \beta(z)\frac{dY}{dz} + \theta Y = 0 \tag{3.4}$$

where $\beta(z) = \{\mu(z) - \frac{1}{4}\sigma^{2\prime}(z)\}/(\sigma^2(z)/2)^{1/2}$

Putting $Y(z) = g(z)y(z)$, where $g(z) = e^{\int_0^z -\frac{1}{2}\beta(u)du}$ gives

$$\frac{d^2y}{dz^2} + (\theta - q(z))y = 0 \tag{3.5}$$

where $q(z) = \frac{1}{4}\beta^2(z) + \frac{1}{2}\beta'(z)$, and with boundary conditions $y'(0) = 0$ and $y(b) = 0$ with $b = Z(r)$.

The eigenvalues of (3.5) are the same eigenvalues as those of (3.4) and (3.2) . Moreover the eigenfunctions of (3.5) are easily transformed into those of (3.2) . In particular if $\psi_n(x)$ is the eigenvalue corresponding to α_n for (3.5) , then $\phi_n(x) = g(Z(x))\psi_n(Z(x))$.

The following powerful asymptotic results (as $n \to \infty$) are known about the eigenvalues and eigenfunctions of the standardized problem (cf [10, p. 19]).

$$\alpha_n = n^2\pi^2/b^2 + 0(1) \tag{3.6}$$

$$\psi_n(x) = (2/b)^{1/2}cos(n\pi x/b) + 0(\frac{1}{n}) \tag{3.7}$$

$$\psi'_n(x) = -n(2/b^3)^{1/2}sin(n\pi x/b) + 0(1) \tag{3.8}$$

4. Obtaining First Passage Moments

To solve (2.1) we need to produce the moment-sequence $\{M_k(x,r)\ ,\ 1 \le k \le n\}$, three such methods are outlined below.

4.1 Complex Integration To Invert Moment Generating Function

Corollary 6.4 shows that $\Psi_\theta(x,r)$ is an analytic function of θ around 0, and so Cauchy's formula implies the identity

$$\frac{M_n(x,r)}{n!} = \frac{1}{2\pi i} \int_{|\theta| = \theta_0} \frac{\Psi_\theta(x,r)}{\theta^{n+1}} d\theta \tag{4.1}$$

where θ_0 is sufficiently small.

The integrals in (4.1) may be computed numerically using Gaussian quadrature to minimize the number of values of θ to be evaluated, and then taking the real part. This reduces evaluating the equation to calculating a small number of values of $\Psi_\theta(x,r)$. Evaluating $\Psi_\theta(x,r)$ may be done by either using finite differences to solve the boundary value problem (cf equation (7.6)), or by using the series method suggested in the differentiation approach, or some hybrid of series and finite differences. An important virtue of estimates of $M_n(x,r)$ based on formula (4.1) is that the accuracy of these estimates is independent of the accuracy of the $n-1$ smaller moments. unlike the methods given in sections (4.2) and (4.3) below.

4.2 Recursive Integration

This approach iteratively uses (6.1) to compute successive moments. This is feasible when the successive moments form a closed family of integrals (compare example 1), or when only a few moments are desired.

Example 1

Choosing parameters $\sigma^2(x) = 2(x + \sigma_0)$ and $\mu(x) = \nu$ where $\nu \neq 0$

gives rise to the iteration:

$$M_n(x) = \int_x^r \frac{n}{(w + \sigma_0)^\nu} \int_0^w M_{n-1}(u)(u + \sigma_0)^{\nu-1} du dw$$

An easy induction will show that for ν not integer $M_{n-1}(x)$ satisfies the expansion

$$M_{n-1}(x) = c[n,0] + \sum_{k=1}^{n} c[n,k](x+a)^k + \sum_{k=1}^{n} d[n,k](x+a)^{k-\nu}$$

where the coefficients are calculated using the iteration:

$c[n,k] = -nc[n-1,k-1]/(k(k-1)+\nu k)$ *where* $k \geq 1$

$d[n,k] = -nd[n-1,k-1]/((-\nu+k)(-\nu+k-1)+\nu(-\nu+k))$ *where* $k \geq 2$

Finally $c[n,0]$ and $d[n,1]$ are determined by solving the two-dimensional linear system arising from the boundary conditions $M_n(r) = 0$ and $M_n'(0) = 0$.

For integer ν , closed formulas for all moments are obtainable, but the calculations will be messier.

4.3 Differentiating the Moment Generating Function

Successive moments may be obtained by calculating the θ-derivatives of the moment generating function $\Psi_\theta(x,r)$ at $\theta = 0$. This approach is facilitated by Kent's observation in [7] that $\Psi_\theta(x,r) = \Upsilon_\theta(x)/\Upsilon_\theta(r)$ where $\Upsilon_\theta(x)$ satisfies

$$\frac{1}{2}\sigma^2(x)\Upsilon_\theta''(x) + \mu(x)\Upsilon_\theta'(x) + \theta\Upsilon_\theta(x) = 0 \tag{4.2}$$

with initial conditions

$$\Upsilon_\theta'(0) = 0 \quad , \quad \Upsilon_\theta(0) \neq 0 \tag{4.3}$$

To solve for the θ-derivatives of $\Psi_\theta(x,r)$ it suffices to solve for the derivatives of $\Upsilon_\theta(x)$. We can obtain $\Upsilon_\theta(x)$ using the series expansion method around x=0 to solve (4.2) . Under certain regularity conditions, the Taylor series coefficients may be differentiated with respect to θ , and the series summed. This process is illustrated in Example 2 below.

Example 2

We indicate how the technique in (4.3) may be applied to Example 1:

$$\Upsilon_\theta(x) = \sum_{j=0}^{\infty} b_j(\theta)x^j$$

Equation (4.2) implies that

$$\sigma^2(x) \sum_{j=0}^{\infty} \binom{j+2}{2} b_{j+2}(\theta)x^j + \mu(x) \sum_{j=0}^{\infty} (j+1)b_{j+1}(\theta)x^j + \theta \sum_{j=0}^{\infty} b_j(\theta)x^j = 0$$

Since $\mu(x) = \nu$ and $\sigma(x) = 2(x+\sigma_0)$ we deduce that

$$\theta b_j(\theta) + (\nu+j(j+1))b_{j+1}(\theta) + \sigma_0(j+2)(j+1)b_{j+2}(\theta) = 0 \text{ for } j \geq 1 \tag{4.4}$$

where the boundary conditions are

$b_0(\theta) = 1$ and $b_1(\theta) = 0$

Repeatedly differentiating (4.4) will give successive iterative formulas for computing $\Upsilon_\theta^{(n)}(x)$. For example for $n=1$

$$\theta b_j'(\theta) + b_j(\theta) + (\nu + j(j+1))b_{j+1}'(\theta) + \sigma_0(j+2)(j+1)b_{j+2}'(\theta)$$

With initial conditions $b_0'(\theta) = b_1'(\theta) = 0$.

If the above iteration diverges, we can always try renormalizing by x and calculating $b_j^{(n)}(\theta)x^n$. If r is sufficiently small then renormalization will suffice, otherwise $\Upsilon_\theta(x)$ can be calculated by successively moving out from 0 towards r as suggested in section (5.1) below, and then using the contour integration method suggested in section (4.1).

5. Some Remarks About Computing $\Psi_\theta(x,r)$

5.1 Computing $\Psi_\theta(0,r)$

The series expansion method may not permit solving for $\Psi_\theta(0,r)$ in a single step. However, suppose the series converges for some $y \in (0,r)$, ie, it is possible to compute $\Psi_\theta(0,y)$ by the series method. We may use $\Psi_\theta(0,y)$ as a bootstrap to calculate $\Psi_\theta(y,r)$ as follows. Observe that $\Psi_\theta(0,r) = \Psi_\theta(0,y)\Psi_\theta(y,r)$. Thus

$$\Psi_\theta(y,r) = -\frac{\Psi_\theta(0,y)}{\frac{\partial \Psi_\theta(0,y)}{\partial y}} \frac{\partial \Psi_\theta(y,r)}{\partial y}$$

Using this initial condition and Kent's normalization technique, it is possible to calculate $\Psi_\theta(y,r)$ starting from y rather than from 0.

5.2 Interpolating $\Psi_\theta(x,r)$ And A Related Boundary Value Problem

Suppose that $\Psi_\theta(x,r)$ and $\Psi_\theta(y,r)$ have been obtained $(x < y)$, and it is desired to calculate $\Psi_\theta(z,r)$ for $z \in (x,y)$. The multiplicative character of $\Psi_\theta(x,r)$ implies that

$$\Psi_\theta(z,r) = \Psi_\theta(z,y)\Psi_\theta(y,r)$$

It thus suffices to determine $\Psi_\theta(z,y)$. We have $\Psi_\theta(x,y) = \Psi_\theta(x,r)/\Psi_\theta(y,r)$ and $\Psi_\theta(y,y) = 1$. Therefore it suffices to find $h_\theta(z)$ ($\equiv$ $\Psi_\theta(z,y)$) such that

$$\frac{1}{2}\sigma^2(z)h_\theta''(z) + \mu(z)h_\theta'(z) + \theta h_\theta(z) = 0 \tag{5.1}$$

with boundary conditions $h_\theta(x) = \Psi_\theta(x,r)/\Psi_\theta(y,r)$ and $h_\theta(y) = 1$. These boundary conditions uniquely determine h_θ . To solve for h_θ , first find ξ_0 and ξ_1 satisfying (5.1) , where $\xi_i'(x) = 1-i$ and $\xi_i(x) = i$, for $i = 0, 1$. Then set

$$h_\theta(z) = \Psi_\theta(x,y)\xi_1(z) + \xi_0(z)(1 - \Psi_\theta(x,y)\xi_1(y))/\xi_0(y)$$

6. Theoretical Complements

In this section some of the properties of moments of τ_x are examined, but first some new notation is introduced.

Define $M_n(x,y) \equiv E^x(\tau_y^n)$ for $x \leq y$ and $n \geq 0$, and let

$$M_n'(x,y) = \frac{\partial M_n(x,y)}{\partial x}$$

$$M_n''(x,y) = \frac{\partial^2 M_n(x,y)}{\partial x^2}$$

6.1 Recursive Equations For Moments Of τ_x

The functions $M_n(x,y)$ jointly satisfy the iterative differential equation (cf [5], p. 203, equation (3.38)).

$$\frac{1}{2}\sigma^2(x)M_n''(x,y) + \mu(x)M_n'(x,y) + nM_{n-1}(x,y) = 0 \tag{6.1}$$

subject to $M_n'(0,y) = 0$ and $M_n(y,y) = 0$.

6.2 Lipschitz Conditions For Moments Of τ_x

Lemma

$M_n(x,y)$ is a smooth function in x and y jointly , and there exists a constant C such that

$$|M_n(x,y)| \leq C^n y^{2n-1}(y-x)n! \tag{6.2}$$

and

$$|M_n'(x,y)| \leq C^n y^{2(n-1)}n!$$

for all $x \leq y$.

Proof:

Set

$$s(x) = \exp\{-\int_0^x \frac{2\mu(\xi)}{\sigma^2(\xi)}\, d\xi\}$$

and

$$m(x) = 1/[\sigma^2(x)s(x)] \ .$$

Rewriting (6.1) as follows

$$\frac{d}{dx}\left(\frac{M_n'(x,y)}{s(x)}\right) = -2nM_{n-1}(x,y)m(x)$$

implies that

$$M_n(x,y) = 2n\int_x^y \left[\int_0^\eta M_{n-1}(\xi,y)m(\xi)d\xi\right]s(\eta)d\eta$$

By virtue of continuity there exists a constant K such that

$$\|s\| \equiv \sup_{0 \le x \le r} |s(x)| \le K$$

and

$$\|m\| \le K \ .$$

Therefore

$$|M_n(x,y)| \le 2n\int_x^y \int_0^\eta K^2 \|M_{n-1}\| d\xi d\eta$$

$$= 2n \ K^2 \|M_{n-1}\| y(y-x) \le 2K^2 y^2 n \, \|M_{n-1}\|$$

An easy induction implies that $M_n(x,y)$ is a smooth function in x and y . moreover

$$\|M_n(x,y)\| \le 2^n K^{2n} y^{2n-1}(y-x)n! \qquad (6.3)$$

and

$$\|M_n'(x,y)\| \le 2^n K^{2n} y^{2(n-1)} n!$$

Taking $C = (2K^2)$ completes the proof.

(6.4) Corollary

$\Psi_\theta(x,y) < \infty$ whenever $|\theta| < C^{-1}y^{-2}$, and

$$\Psi_\theta(x,y) = \sum_{n=0}^{\infty} \frac{\theta^n}{n!} M_n(x,y) \qquad (6.4)$$

6.3 Infinitesimal Relations Governing First Passage Moments

Proposition

Define

$$U_n(x,y) \equiv \frac{\partial M_n(x,y)}{\partial y}$$

and

$$u_n(x) \equiv U_n(x,x)$$

Then $M_n(x,y)$, $U_n(x,y)$, $u_n(x)$ satisfy

$$M_n(0,y) = \sum_{j=0}^{n} \binom{n}{j} M_j(0,x) M_{n-j}(x,y) \qquad (6.5)$$

$$U_n(0,x) = \sum_{j=0}^{n-1} \binom{n}{j} M_j(0,x) u_{n-j}(x) \qquad (6.6)$$

Proof

Conditional on $X(0) = 0$ the strong Markov property **(SMP)** implies that $\{ \tau_{a_1}, \tau_{a_2} - \tau_{a_1}, \ldots, \tau_r - \tau_{a_n} \}$, where $0 < a_1 < a_2 < \cdots < a_n < r$, form a set of independent random variables. In particular

$$\begin{aligned} M_n(0,y) \equiv E^0[\tau_y^n] &= E^0[(\tau_x + \tau_y - \tau_x)^n] \\ &= \sum_{j=0}^{n} \binom{n}{j} E^0[\ \tau_x)^j\ (\tau_y - \tau_x)^{n-j}\ ] \\ &= \sum_{j=0}^{n} \binom{n}{j} E^0[\ \tau_x)^j\ ]\ E^x[(\tau_y - \tau_x)^{n-j}\ ] \end{aligned}$$

which coincides with (6.5) . Using a little algebraic manipulation on (6.5) shows that

$$[M_n(0,y) - M_n(0,x)]/(y-x) = \sum_{j=0}^{n-1} \binom{n}{j} M_j(0,x) M_{n-j}(x,y)/(y-x) \qquad (6.7)$$

Now letting $y \rightarrow x$ in (6.7) yields (6.6) . QED

Comments

Equations (6.5) and (6.6) provide sor nice intuition about the way that first passage times from x to y depend on fi. passage times from 0 to x.

Equations (6.5) and (6.6) are similar to (6.1) , but may capture better the dependence of higher moments on lower moments. From a practical point of view equation (6.1) is certainly preferable for moment calculation. In section 4, other methods are proposed for calculating the moments $M_n(x,y)$.

7. A Representation Result

Theorem

$$\Psi_\theta(x,y) = \exp\{ \sum_{n=1}^{\infty} \int_x^y u_n(z) \ \frac{\theta^n}{n!} dz \} \tag{7.1}$$

where $\{u_n(z) \ , \ n \geq 1\}$ satisfy

$$\frac{1}{2}\sigma^2(x) u_1{}'(x) + \mu(x) u_1(x) = 1 \ , \tag{7.2}$$

and for $n \geq 2$

$$\frac{1}{2}\sigma^2(x) u_n{}'(x) + \mu(x) u_n(x) = \frac{1}{2}\sigma^2(x) \sum_{k=1}^{n-1} \frac{u_k(x) u_{n-k}(x)}{k!(n-k)!} \tag{7.3}$$

Proof

We begin by showing that (7.1) holds for $\Psi_\theta(0,r)$.

Let $x_j = jr/L$ for $0 \leq j \leq L$. Using the **SMP** as in the proof of (6.5),

$$\Psi_\theta(0,r) = \prod_{j=0}^{L-1} \Psi_\theta(x_j, x_{j+1})$$

Taking logarithms.

$$\log \Psi_\theta(0,r) = \sum_{j=0}^{L-1} \log \Psi_\theta(x_j, x_{j+1})$$

Applying proposition (8.4) to the above yields

$$\log \Psi_\theta(0,r) = \sum_{j=0}^{L-1} [\Psi_\theta(x_j, x_{j+1}) - 1 + (\Psi_\theta(x_j, x_{j+1}) - 1)^2 g(\Psi_\theta(x_j, x_{j+1}))] \ .$$

Since $\Psi_\theta(x,x) = 1$ it follows

$$\Psi_\theta(x_j, x_{j+1}) - 1 = \frac{\partial \Psi_\theta}{\partial y}(x_j, x_j + \alpha L^{-1}) \ L^{-1}$$

where $0 < \alpha < 1$. Also since $\Psi_\theta(x,y)$ is a smooth function in x and y jointly , it follows that $\frac{\partial \Psi_\theta(x,y)}{\partial y}$ is uniformly bounded on the region $0 \leq x \leq y \leq r$. So there exists a function $h(L)$ such that $h(L) \sim O(1)$

$$\log \Psi_\theta(0,r) = \sum_{j=0}^{L-1} [\Psi_\theta(x_j, x_{j+1}) - 1] + h(L) L^{-1} \ .$$

Replacing each $\Psi_\theta(x_j,x_{j+1})$ in the above by the expression in (6.4), yields

$$\log\Psi_\theta(0,r) = \sum_{j=0}^{L-1}\sum_{n=1}^{\infty} \frac{\theta^n M_n(x_j,x_{j+1})}{n!} + O(L^{-1})$$

Since the summands are positive the order of summation may be permuted to get

$$\log\Psi_\theta(0,r) = \sum_{n=1}^{\infty}\sum_{j=0}^{L-1} \frac{\theta^n M_n(x_j,x_{j+1})}{n!} + O(L^{-1})$$

The inner summation can be expressed as a Riemann sum

$$\log\Psi_\theta(0,r) = \sum_{n=1}^{\infty} \theta^n \sum_{j=0}^{L-1} \frac{M_n(x_j,x_{j+1})}{n!\, L^{-1}} \frac{1}{L} + O(L^{-1}) \tag{7.4}$$

Equation (6.2) implies that

$$\frac{M_n(x_j,x_{j+1})}{n!\, L^{-1}} \le C^n (x_{j+1})^{2n} \le C_0{}^n .$$

where $C_0 = Cr^2$.

The Lebesgue dominated convergence theorem (applied to the product space $\{1,2,..\} \times [0,r]$ endowed with product of the counting measure with the Lebesgue measure on [0,r]) implies the right side of (7.4) approaches the limit

$$\log\Psi_\theta(0,r) = \sum_{n=1}^{\infty} \frac{\theta^n}{n!} \int_0^r u_n(z)dz$$

as $L \to \infty$, or

$$\Psi_\theta(0,r) = \exp\{ \sum_{n=1}^{\infty} \frac{\theta^n}{n!} \int_0^r u_n(z)\, dz\}$$

Due to the multiplicative nature of $\Psi_\theta(x,y)$ it is easy to show that

$$\Psi_\theta(x,y) = \exp\{ \sum_{n=1}^{\infty} \int_x^y u_n(z) \frac{\theta^n}{n!} dz\} \tag{7.5}$$

The function $\Psi_\theta(x,y)$ satisfies the following differential equation (cf [5] pp 203)

$$\frac{1}{2}\sigma^2(x)\frac{\partial^2\Psi_\theta(x,y)}{\partial x^2} + \mu(x)\frac{\partial\Psi_\theta(x,y)}{\partial x} + \theta\Psi_\theta(x,y) = 0 \tag{7.6}$$

subject to $\dfrac{\partial \Psi_\theta(0,y)}{\partial x} = 0$ and $\Psi_\theta(y,y) = 1$.

Substituting equation (7.5) in (7.6) , shows that the exponent in (7.5) satisfies the differential equation

$$\frac{1}{2}\sigma^2(x)[(\sum_{n=1}^{\infty} \frac{\theta^n}{n!} u_n(x))^2 \;-\; \sum_{n=1}^{\infty} \frac{\theta^n}{n!} u_n{}'(x)] \;-\; \mu(x) \sum_{n=1}^{\infty} \frac{\theta^n}{n!} u_n(x)] + \theta \;=\; 0 \,.$$

Since the above series converge absolutely for θ sufficiently small, we can rearrange terms to obtain a single power series in θ . Since this power series is zero for θ sufficiently small, all its coefficients must be zero. Setting the coefficients of θ to zero yields equations (7.2) and (7.3) .

The initial condition that $\dfrac{\partial \Psi_\theta(0,y)}{\partial x} = 0$ in (7.6) implies

$u_n(0) = 0$, *where* $n \geq 1$.

8. Appendix

8.1 Spectral Representations For First Passage Time Distributions

Theorem The right-hand-side of (1.3) is the unique function satisfying (1.2), jointly continuous in x and t on $[0,r] \times (0,\infty)$ with $\dfrac{\partial w(x,t)}{\partial t}$ absolutely integrable over $[0,r] \times (N^{-1}, N)$ for all $N \geq 1$.

Proof:
Suppose that w(x,t) satisfies equation (1.2) and the integrability conditions. Observe that for fixed $t > 0$ $w(x,t)$ is a continuous function of x belonging to $L^2(\rho)$. Therefore $w(x,t)$ possesses the orthogonal expansion

$$w(x,t) = \sum_{k=1}^{\infty} c_k(t)\ \phi_k(x)$$

where

$$c_k(t) = \int_0^r w(x,t)\ \phi_k(x)\rho(x)dx$$

Multiply (1.2) by $\phi_k(x)$ and integrate over $[0,r]$ to get

$$\int_0^r \frac{\partial w(x,t)}{\partial t}\ \phi_k(x)\rho(x)dx = \int_0^r Aw(x,t)\phi_k(x)\rho(x)dx\ .$$

Now since $Af(x)\rho(x) = \pi(x)f''(x) + \pi'(x)f'(x)$ (cf (3.1) and (3.2)), a simple integration by parts shows

$$\int_0^r Aw(x,t)\phi_k(x)\rho(x)dx = \int_0^r w(x,t)A\,\phi_k(x)\rho(x)dx$$

The relationship $A\,\phi_k(x) = -\alpha_k\phi_k(x)$ implies that

$$\int_0^r \frac{\partial w(x,t)}{\partial t}\phi_k(x)\rho(x)dx = -\int_0^r \alpha_k w(x,t)\phi_k(x)\rho(x)dx\ .$$

Integrating both sides with respect to t over $[u_0,u]$ and permuting the order of integration on the left-hand-side yields (permissible because Fubini's Theorem applies to the absolutely integrand $\dfrac{\partial w(x,t)}{\partial t}\phi_k(x)\rho(x)$).

$$\int_0^r \int_{u_0}^u \frac{\partial w(x,t)}{\partial t}\phi_k(x)\rho(x)\ dt\ dx = \int_{u_0}^u \int_0^r -\alpha_k w(x,t)\phi_k(x)\rho(x)\ dx\ dt$$

Using the definition of $c_k(t)$ on the right-hand-side of the last equation implies

$$c_k(u) + C = \int_{u_0}^{u} c_k(t)dt ,$$

where C is an arbitrary constant.

Therefore $c_k(t) = c_k e^{-\alpha_k t}$. It remains to determine the constants c_k , but they may be derived from the boundary condition $w(x,0) = 1$ for $0 < x < r$ as follows. Since ρ is continuous, $w(x,0) = 1$ for almost all $\rho(dx)$, and $1 \in L^2(\rho)$. So

$$1 = \sum_{k=1}^{\infty} c_k \phi_k(x) \tag{8.1}$$

where

$$c_k = \int_0^r \phi_k(x)\rho(x)dx \tag{8.2}$$

Now Theorem 1.9 of [10] implies that the right-hand-side of (8.1) converges pointwise to 1 on $(0,r)$. Therefore $w(x,t)$ has the representation

$$w(x,t) = \sum_{k=1}^{\infty} c_k \, e^{-\alpha_k t} \phi_k(x) \tag{8.3}$$

To prove the converse, suppose that $w(x,t)$ is defined by (8.2) and (8.3) jointly. Equations (3.7) and (8.2) imply that the coefficients c_k , $k \geq 1$ are uniformly bounded. Hence for $t > \epsilon > 0$ the series converges uniformly to a function continuous on the product $[0,r] \times [\epsilon,\infty)$. The uniform convergence and boundary conditions on the eigenfunctions imply the boundary conditions on x . The integrability conditions on $\frac{\partial w(x,t)}{\partial t}$ follow in similar fashion. The boundary condition $w(x,0) = 1$ for $x \in (0,r)$ follows from Theorem 1.9 of [10] and equation (8.1) The differential equation (1.2) may be derived from the definition of derivatives as limits of divided differences, and the dominated convergence theorem applied to series. QED.

It should be noted that the first passage time distribution satisfies the regularity conditions of the theorem, and therefore must have representation (1.2).

8.2 Convergence Of The Finite Approximations To The Infinite Vector

It will now be shown that the solution vector to system (2.1) , denoted by

$\mathbf{p}^{(n)} = \{p_k^{(n)}, 1 \le k \le n\}$, converges at rate n^{-2} component-wise to the infinite vector $\mathbf{p} = \{p_k, k \ge 1\}$, where $p_k = c_k \phi_k(x)$.

Theorem

$$|p_k^{(n)} - p_k| = O(\frac{1}{n^2})$$

Proof: Define $\nu_k^{(n)}$, $\delta_k^{(n)}$ and $\eta_k^{(n)}$ as follows:

$$\nu_k^{(n)} = \sum_{j=1}^{n} \mu_j^k p_j \quad where \ 0 \le k \le n-1$$

$$\delta_k^{(n)} = m_k - \nu_k^{(n)} = \sum_{j=n+1}^{\infty} \mu_j^k p_j \quad where \ 0 \le k \le n-1 \tag{8.4}$$

$$\eta_k^{(n)} = p_k - p_k^{(n)}$$

Observe that $\{\nu_k^{(n)}, 1 \le k \le n\}$ is the solution to (2.2) where $\{m_n, 1 \le k \le n\}$ has been replaced by $\{\delta_k^{(n)}, 1 \le k \le n\}$. In particular

$$\nu_k^{(n)} = \sum_{1 \le j \le n} \delta_j^{(n)} g_{n-j}(\mu_1,\mu_2, \cdots ,\mu_{k-1}, \mu_{k+1}, \cdots \mu_n) \Big/ \prod_{\substack{1 \le j \le n \\ j \ne k}} (\mu_j - \mu_k) \tag{8.5}$$

For $1 \le j \le n$

$$|g_{n-j}((\mu_1,\mu_2, \cdots ,\mu_{k-1}, \mu_{k+1}, \cdots \mu_n))| \le \mu_k^{n-j-k}$$

Also equations (3.2), (3.6) and (3.7) together imply that $|c_n| = O(\frac{1}{n})$, thus (8.4) and (3.6) imply

$$|\delta_j^{(n)}| \le C n^{-2j}$$

So

$$\left|\sum_{j=1}^{n} g_{n-j}((\mu_1,\mu_2, \cdots ,\mu_{k-1}, \mu_{k+1}, \cdots \mu_n))\delta_j^{(n)}\right| \le \sum_{j=1}^{n} \mu_k^{n-j-k}|\delta_j^{(n)}|$$

$$\le \mu_k^{n-k} \sum_{j=1}^{k} C n^{-2j} \mu_k^{-j} = \mu_k^{n-k-1} 0(\frac{1}{n^2})$$

Thus

$$\left|\sum_{j=1}^{n} g_{n-j}((\mu_1,\mu_2, \cdots ,\mu_{k-1}, \mu_{k+1}, \cdots \mu_n))\delta_j^{(n)}\right| = 0(\frac{\mu_k^{n-k-1}}{n^2})$$

Finally, the denominator of (8.5) may be written as

$$\prod_{\substack{1 \le j \le n \\ j \ne k}} (\mu_j - \mu_k) = \mu_k^{n-k} d_k^{(n)}$$

where

$$d_k^{(n)} = \prod_{1 \le j \le k-1} (\mu_j - \mu_k) \prod_{k+1 \le j \le n} (1 - \frac{\mu_j}{\mu_k})$$

Now equation (3.6) and the Weierstrass Product Convergence test jointly imply that

$$\lim_{n \to \infty} d_k^{(n)} = d > 0$$

Now it follows that $\eta_k^{(n)} = O(\frac{1}{n^2})$ as claimed.

8.3 A Conjecture

It is interesting to note that $p_k(x)$ is linearly proportional to the eigenfunction $\phi_k(x)$. and therefore $Ap_k(x) = \alpha_k p_k(x)$. This suggests that $p_k^{(n)}(x)$ will approximately satisfy this relation. Observe that $Am_k(x) = -m_{k-1}(x)$. Thus

$$Ap_k^{(n)}(x) = \sum_{1 \le j \le n-1} -m_j g_{n-j-1}(\mu_1, \mu_2, \cdots, \mu_{k-1}, \mu_{k+1}, \cdots \mu_n) \Big/ \prod_{\substack{1 \le j \le n \\ j \ne k}} (\mu_j - \mu_k)$$

Comparing this with (2.3) suggests that

$$\lim_{n \to \infty} \frac{g_{n-j-1}((\mu_1, \mu_2, \cdots, \mu_{k-1}, \mu_{k+1}, \cdots \mu_n))}{g_{n-j}((\mu_1, \mu_2, \cdots, \mu_{k-1}, \mu_{k+1}, \cdots \mu_n))} = \alpha_k = \frac{1}{\mu_k}$$

8.4 Proposition

For $1 \le x < 2$

$$|log(x) - x + 1| = (x-1)^2 g(x)/2 \text{ , where } |g(x)| < 1$$

Proof: The mean value theorem applied to $log(x)$ at x=1 gives:
$log(x) = log(1+x-1) = log(1) + (x-1) - (x-1)^2/2(1+\alpha(x-1)^{-2})$
where $0 < \alpha < 1$. The prop now follows from $x \ge 1$ and $\alpha > 0$.

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